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# On Certain Degree Based and Bond Additive Molecular Descriptors of Hexabenzocorenene

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**Abstract:** The molecular descriptor is the final number that comes from a numerical method that uses a picture of a structure to turn chemical information into a useful number. The structure-based investigations revealed a close link between topological structures and their physical practices, synthetic properties, and natural traits. Auxiliary descriptors of this type have been effectively used to improve understanding of sub-atomic structures. In this study, the atomic representations of three major classes of polycyclic aromatic hydrocarbons, such as hexa-peri-hexabenzocoronene, are used in a non-experimental graph-theoretic technique that yields the mathematical structural quantities of the substances under consideration.

**Keywords:** molecular graph; topological indices; nanographene; hexabenzocoronene.



## 1. Introduction

Organic intensifiers known as polycyclic aromatic hydrocarbons (PAHs) are colorless, white, or light-yellow solids. They are an all-pervasive assemblage of a few hundred chemically similar molecules, earthly industrious with varying structures and severity. They cause harm to animals through a variety of actions. PAH stands for polycyclic aromatic hydrocarbons, made up of carbon and hydrogen atoms. At least two benzene rings have been strengthened in the PAHs' linear, cluster, or angular orientations. PAHs have high melting and boiling temperatures, low vapor pressures, and insufficient liquid absorption. In the meanwhile, because PAHs are extremely lipophilic, they may be dissolved in natural solvents. PAHs have a variety of properties, including light affectability, heat resistance, conductivity, emittance capacity, erosion resistance, and physiological activity. They are commonly used as intermediaries in medicines, agricultural products, photographic products, thermosetting plastics, lubricating lubricants, and other compound enterprises, according to [1]. Their compounds and molecular structure determine PAHs' chemical and biological properties. Quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) techniques have been developed to predict the characteristics of polycyclic benzenoid compounds and related graphs based on their structures [2-4]. There are various topological indices widely available, some of which are used in chemistry. The structural properties of the graphs used for their computation can be used to classify them. Polycyclic aromatics' chemical and bioactivities are of great interest due to their widespread application in the petroleum sector, chemical manufacture, and pharmaceutical endeavors. As a result, their toxicity, carcinogenicity, and dermal incursions have all received significant attention. Numerous residencies of the understudied molecular compounds may be correlated with degree-based topological indices, which have received substantial investigation.

## 2. Materials and Methods

Hexa-peri-hexabenzocoronene (HBC), or simply hexabenzocoronene [5-8], is a polycyclic aromatic hydrocarbon with the chemical formula $C_{42}H_{18}$. Figure 1 shows a core coronene molecule with an additional benzene ring fused between each neighboring pair of rings surrounding the perimeter [9]. In [10], the synthesis of hexa-peri-hexabenzocoronene was described.

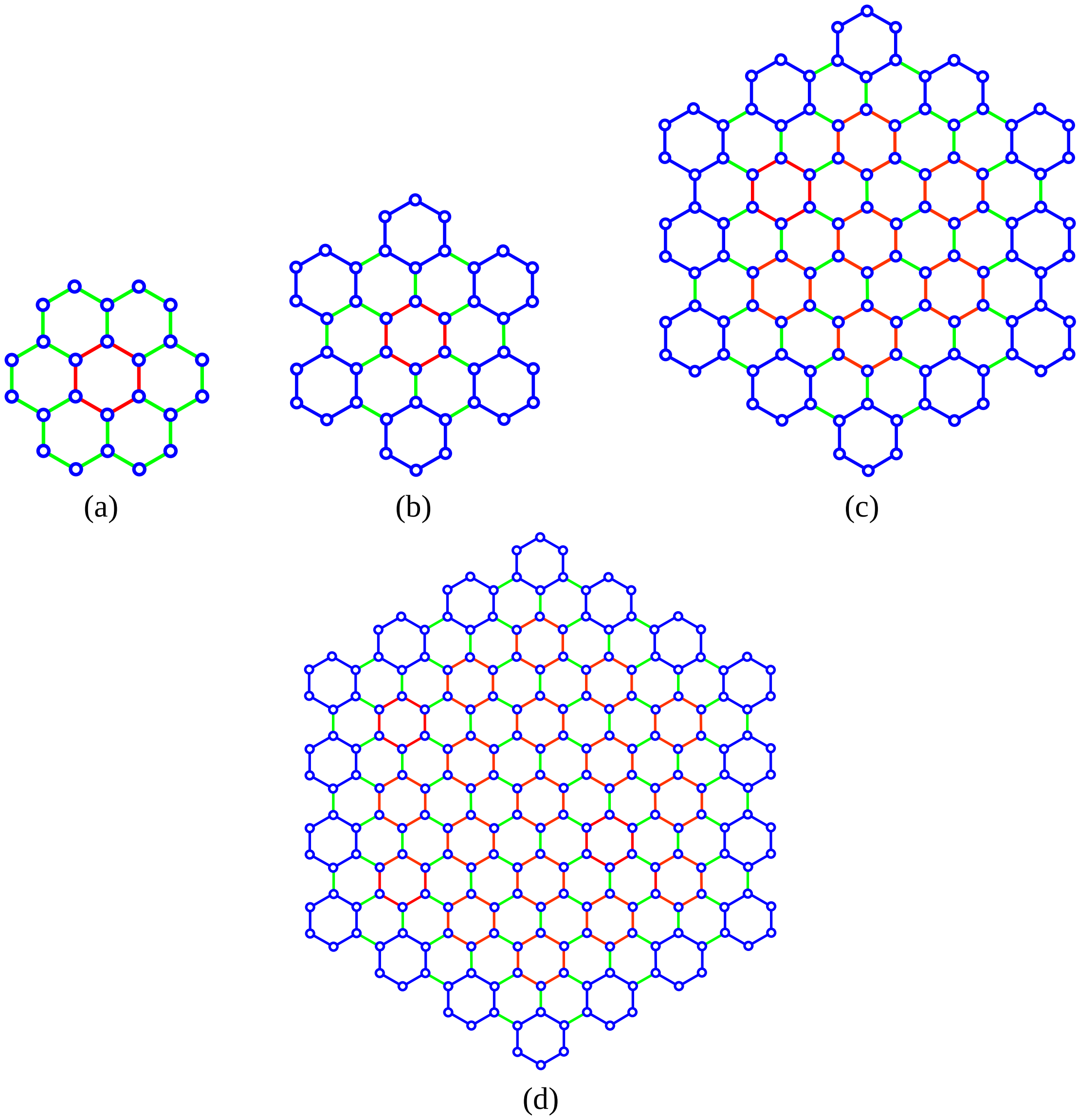


**Figure 1. (a)** Coronene; **(b)** Hexa-cata-hexabenzocoronene ($C_{48}H_{24}$) HBC (2); **(c)** HBC (3); (**d**) HBC (4).

HBC molecules are very stable, having strong intermolecular forces that promote self-assembly. Because of their disc form, HBCs most commonly form columnar structures via $pi-pi$ interaction [11]. HBC may be seen as the smallest form of graphene, with graphene-like characteristics. It is possible to make functionalized HBC derivatives with various characteristics, like fluid crystallinity. On the HBC particle, synthetic flexibility also takes into mind a wide range of practical groupings. As a result, nanostructured materials are predicted to be used in biology, energy storage, and organic electronics. These derivatives have been used in various applications, ranging from sensors and batteries to semiconductors and solar cells.

Let $G=(V(G),E(G))$ be a molecular graph. The cardinality of these sets denotes the number of vertices and edges correspondingly. An edge in $E(G)$ with end vertices $u$ and $v$ is indicated as $e=uv$. If there is a path between two vertices $u$ and $v$, they are said to have been adjacent. Computational chemistry is a field of material science in which we use mathematical models to explore and identify chemical structures without necessarily using quantum mechanics. Chemical graph theory [12,13] is a field of mathematical chemistry that attempts to use graph theory in the mathematical modeling of chemical processes. This theory had an important effect on the development of the chemical sciences.

A topological descriptor is a mathematical number associated with a molecular structure that describes the link between that structure and a range of physical attributes, chemical reactivity, or biological activity. Quantitative structure-activity and structure-property interaction imply representations of the topological properties of the chemical structure. Chemical graph theory is used in QSAR to represent hydrogen-exhausted graphs of organic chemical networks, where the points correspond to the vertices and edges of the unique chemical component's bonds. The topological division of quantitative chemistry that applies the graph hypothesis to the numerical study of chemical processes is known as the chemical graph hypothesis. The supporters of the theory retain the qualities of a chemical graph, that is, a graph of a hypothetical demonstration of a particle that provides important insight into the substance's phenomena. A molecular graph is commonly used to represent molecules and chemical compounds. Topological indices are useful tools supplied by graph theory for learning about hypothetical material compounds. [14-48].

### *2.1. Various degree-based topological indices.*

**Table 1**. Degree-based topological indices of Hexa-peri-hexabenzocoronene (HBC).

| **Topological Indices [14-17]** | **Mathematical Expressions** |
|---|---|
| Randic$'$ | $R(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d(u)d(v)}}$ |
| Reciprocal Randic$'$ | $RR(G)=\sum_{uv\in E(G)}\sqrt{d(u)d(v)}$ |
| Reduced reciprocal Randic$'$ | $RRR(G)=\sum_{uv\in E(G)}\sqrt{(d(u)-1)(d(v)-1)}$ |
| First Zagreb | $M_1(G)=\sum_{u\in V(G)}d(u)^2$ |
| Second Zagreb | $M_2(G)=\sum_{uv\in E(G)}d(u)d(v)$ |
| Reduced Second Zagreb | $RM_2(G)=\sum_{uv\in E(G)}(d(u)-1)(d(v)-1)$ |
| Hyper Zagreb | $HM(G)=\sum_{uv\in E(G)}[d(u)+d(v)]^2$ |

| Topological Indices [14-17] | Mathematical Expressions |
|---|---|
| Augmented Zagreb | $AZ(G)=\sum_{uv\in E(G)}\left(\frac{d(u)d(v)}{d(u)+d(v)-2}\right)^3$ |
| Atom bond connectivity | $ABC(G)=\sum_{uv\in E(G)}\sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$ |
| Harmonic | $H(G)=\sum_{uv\in E(G)}\frac{2}{d(u)+d(v)}$ |
| Sum-connectivity | $SC(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d(u)+d(v)}}$ |
| Geometric arithmetic | $GA(G)=\sum_{uv\in E(G)}2\left(\frac{\sqrt{d(u)d(v)}}{d(u)+d(v)}\right)$ |
| Inverse sum index | $ISI(G)=\sum_{uv\in E(G)}\left(\frac{d(u)d(v)}{d(u)+d(v)}\right)$ |

*2.2. Bond additive descriptors.*

Many descriptors are bond additive; they can be presented as a sum of edge contributions. A bond additive descriptor *Des* can be written as [49]

$$Des(G)=\sum_{uv\in E(G)} f(d_G(u),d_G(v)).$$

Where $\boldsymbol{E(G)}$ is the set of edges and $\boldsymbol{f}$ is a mapping that assigns a real value to an ordered pair consisting of a graph and its edge. It can be seen that this is a quite general definition since $\boldsymbol{f}$ can be determined in many ways.

**Table 2.** Adriatic indices and their relavance.

| S. No | Index | $f(d_G(u),d_G(v))$ | Relavance |
|---|---|---|---|
| 1 | Randic$'$ type lordeg index | $ln(d_u)ln(d_v)$ | Heat capacity at constant T for octane isomers |
| 2 | Sum lordeg index | $\sqrt{ln(d_u)}+\sqrt{ln(d_v)}$ | Octanol-water partition coefficient for octane isomers |
| 3 | inverse sum lordeg index | $\frac{1}{\sqrt{ln(d_u)}+\sqrt{ln(d_v)}}$ | Heat capacity at constant P and total surface area for octane isomers |
| 4 | Misbalance lordeg index | $\lvert lnd_u-lnd_v\rvert$ | Standard enthalpy of vaporization for octane isomers, also enthalpy of vaporization for octane isomers. |
| 5 | Misbalance losdeg index | $\lvert ln^2d_u-ln^2d_v\rvert$ | Standard enthalpy of vaporization for octane isomers |
| 6 | Misbalance indeg index | $\lvert\frac{1}{d_u}-\frac{1}{d_v}\rvert$ | Standard enthalpy of vaporization for octane isomers |
| 7 | Misbalance irdeg index | $\lvert\frac{1}{\sqrt{d_u}}-\frac{1}{\sqrt{d_v}}\rvert$ | Enthalpy of vaporization and standard enthalpy of vaporization for octane isomers |
| 8 | Misbalance rodeg index | $\lvert\sqrt{d_u}-\sqrt{d_v}\rvert$ | Enthalpy of vaporization and standard enthalpy of vaporization for octane isomers |
| 9 | Misbalance deg index | $\lvert d_u-d_v\rvert$ | Standard enthalpy of vaporization for octane isomers |
| 10 | Misbalance hadeg index | $\lvert\left(\frac{1}{2}\right)^{d_u}-\left(\frac{1}{2}\right)^{d_v}\rvert$ | Enthalpy of vaporization and standard enthalpy of vaporization for octane isomers |
| 11 | Min-max rodeg index | $\sqrt{\frac{min(d_u,d_v)}{max(d_u,d_v)}}$ | Standard enthalpy of vaporization for octane isomers |
| 12 | Max-min rodeg index | $\sqrt{\frac{max(d_u,d_v)}{min(d_u,d_v)}}$ | Enthalpy of vaporization for octane isomers, enthalpy of vaporization for octane isomers, and log water activity coefficient for polychlorobiphenyls. |
| 13 | Max-min deg index | $\frac{max(d_u,d_v)}{min(d_u,d_v)}$ | Log water activity coefficient for polychlorobiphenyls |
| 14 | Max-min sdeg index | $\left(\frac{max(d_u,d_v)}{min(d_u,d_v)}\right)^2$ | Log water activity coefficient for polychlorobiphenyls |

| S. No | Index | $f(d_G(u), d_G(v))$ | Relavance |
|---|---|---|---|
| 15 | Symmetric division deg index | $\frac{min(d_u, d_v)}{max(d_u, d_v)} + \frac{max(d_u, d_v)}{min(d_u, d_v)}$ | Total surface area for polychlorobiphenyls |

## 3. Various Degree Based Topological Indices of Hexa-peri-hexabenzocoronene (HBC)

*3.1 Hexa-peri-hexabenzocoronene (HBC).*

There are $12n - 6$ vertices of degree 2, $18n^2 - 30n + 12$ vertices of degree 3. The edge partition is presented in Table 3.

**Table 3.** The Edge partition of Hexa-peri-hexabenzocoronene (HBC).

| S. No | Edge Type | $(d(u), d(v))$ | Frequency |
|---|---|---|---|
| 1 | $E_1$ | (2,2) | $6n$ |
| 2 | $E_2$ | (2,3) | $12n - 12$ |
| 3 | $E_3$ | (3,3) | $27n^2 - 51n + 24$ |

Theorem 3.1 Let $G$ be a Hexa-peri-hexabenzocoronene (HBC). Then

1. $R(G) = 9n^2 + (2\sqrt{6} - 14)n - 2\sqrt{6} + 8.$
2. $RR(G) = 81n^2 + (12\sqrt{6} - 141)n - 12\sqrt{6} + 72.$
3. $RRR(G) = 54n^2 + (12\sqrt{2} - 96)n - 12\sqrt{2} + 48.$
4. $M_1(G) = 162n^2 - 222n + 84.$
5. $M_2(G) = 243n^2 - 363n + 144.$
6. $RM_2(G) = 108n^2 - 174n + 72.$
7. $HM(G) = 972n^2 - 1440n + 564.$
8. $AZ(G) = \frac{1}{64}[19683n^2 - 27963n + 11352].$
9. $ABC(G) = 18n^2 + (9\sqrt{2} - 34)n - 6\sqrt{2} + 16.$
10. $H(G) = \frac{1}{5}[45n^2 - 46n + 16].$
11. $SC(G) = \frac{1}{\sqrt{30}}[27\sqrt{5}n^2 + (3\sqrt{30} + 12\sqrt{6} - 51\sqrt{5})n - 12\sqrt{6} + 24\sqrt{5}].$
12. $GA(G) = \frac{1}{5}[135n^2 + (24\sqrt{6} - 225)n - 24\sqrt{6} + 120].$
13. $ISI(G) = \frac{1}{10}[405n^2 - 561n + 216].$

Proof.

$$R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d(u)d(v)}}$$
$$= \sum_{i=1}^{3} \sum_{uv\in E_i} \frac{1}{\sqrt{d(u)d(v)}}$$
$$= \frac{1}{\sqrt{2\times2}}(6n) + \frac{1}{\sqrt{2\times3}}(12n - 12) + \frac{1}{\sqrt{3\times3}}(27n^2 - 51n + 24)$$
$$= 9n^2 + (2\sqrt{6} - 14)n - 2\sqrt{6} + 8.$$
$$RR(G) = \sum_{uv\in E(G)} \sqrt{d(u)d(v)}$$
$$= \sum_{i=1}^{3} \sum_{uv\in E_i} \sqrt{d(u)d(v)}$$
$$= (\sqrt{2\times2})(6n) + (\sqrt{2\times3})(12n - 12) + (\sqrt{3\times3})(27n^2 - 51n + 24)$$
$$= 81n^2 + (12\sqrt{6} - 141)n - 12\sqrt{6} + 72.$$
$$RRR(G) = \sum_{uv\in E(G)} \sqrt{(d(u) - 1)(d(v) - 1)}$$

$= \sum_{i=1}^{3} \sum_{uv \in E_i} \sqrt{(d(u)-1)(d(v)-1)}$
$= (\sqrt{1 \times 1})(6n) + (\sqrt{1 \times 2})(12n-12) + (\sqrt{2 \times 2})(27n^2 - 51n + 24)$
$= 54n^2 + (12\sqrt{2} - 96)n - 12\sqrt{2} + 48.$
$M_1(G) = \sum_{u \in V(G)} d(u)^2$
$= (2^2)(12n-6) + (3^2)(18n^2 - 30n + 12)$
$= 162n^2 - 222n + 84.$
$M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$
$= \sum_{i=1}^{3} \sum_{uv \in E_i} d(u)d(v)$
$= (2 \times 2)(6n) + (2 \times 3)(12n-12) + (3 \times 3)(27n^2 - 51n + 24)$
$= 243n^2 - 363n + 144.$
$RM_2(G) = \sum_{uv \in E(G)} (d(u)-1)(d(v)-1)$
$= \sum_{i=1}^{3} \sum_{uv \in E_i} (d(u)-1)(d(v)-1)$
$= (1 \times 1)(6n) + (1 \times 2)(12n-12) + (2 \times 2)(27n^2 - 51n + 24)$
$= 108n^2 - 174n + 72.$
$HM(G) = \sum_{uv \in E(G)} [d(u) + d(v)]^2$
$= \sum_{i=1}^{3} \sum_{uv \in E_i} [d(u) + d(v)]^2$
$= (2+2)^2(6n) + (2+3)^2(12n-12) + (3+3)^2(27n^2 - 51n + 24)$
$= 972n^2 - 1440n + 564.$
$AZ(G) = \sum_{uv \in E(G)} \left(\frac{d(u)d(v)}{d(u)+d(v)-2}\right)^3$
$= \sum_{i=1}^{3} \sum_{uv \in E_i} \left(\frac{d(u)d(v)}{d(u)+d(v)-2}\right)^3$
$= \left(\frac{2\times2}{2+2-2}\right)^3 (6n) + \left(\frac{2\times3}{2+3-2}\right)^3 (12n-12) + \left(\frac{3\times3}{3+3-2}\right)^3 (27n^2 - 51n + 24)$
$= \frac{1}{64}[19683n^2 - 27963n + 11352].$
$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$
$= \sum_{i=1}^{3} \sum_{uv \in E_i} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$
$= \left(\sqrt{\frac{2+2-2}{2\times2}}\right)(6n) + \left(\sqrt{\frac{2+3-2}{2\times3}}\right)(12n-12) + \left(\sqrt{\frac{3+3-2}{3\times3}}\right)(27n^2 - 51n + 24)$
$= 18n^2 + (9\sqrt{2} - 34)n - 6\sqrt{2} + 16.$
$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u)+d(v)}$
$= \sum_{i=1}^{3} \sum_{uv \in E_i} \frac{2}{d(u)+d(v)}$
$= \frac{2}{2+2}(6n) + \frac{2}{2+3}(12n-12) + \frac{2}{3+3}(27n^2 - 51n + 24)$
$= \frac{1}{5}[45n^2 - 46n + 16].$
$SC(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)+d(v)}}$
$= \sum_{i=1}^{3} \sum_{uv \in E_i} \frac{1}{\sqrt{d(u)+d(v)}}$
$= \frac{1}{\sqrt{2+2}}(6n) + \frac{1}{\sqrt{2+3}}(12n-12) + \frac{1}{\sqrt{3+3}}(27n^2 - 51n + 24)$
$= \frac{1}{\sqrt{30}}\left[27\sqrt{5}n^2 + (3\sqrt{30} + 12\sqrt{6} - 51\sqrt{5})n - 12\sqrt{6} + 24\sqrt{5}\right].$

$$GA(G)=\sum_{uv\in E(G)}2\left(\frac{\sqrt{d(u)d(v)}}{d(u)+d(v)}\right)$$
$$=\sum_{i=1}^{3}\sum_{uv\in E_i}2\left(\frac{\sqrt{d(u)d(v)}}{d(u)+d(v)}\right)$$
$$=2\left(\frac{\sqrt{2\times2}}{2+2}\right)(6n)+2\left(\frac{\sqrt{2\times3}}{2+3}\right)(12n-12)+2\left(\frac{\sqrt{3\times3}}{3+3}\right)(27n^2-51n+24)$$
$$=\frac{1}{5}\left[135n^2+\left(24\sqrt{6}-225\right)n-24\sqrt{6}+120\right].$$
$$ISI(G)=\sum_{uv\in E(G)}\left(\frac{d(u)d(v)}{d(u)+d(v)}\right)$$
$$=\sum_{i=1}^{3}\sum_{uv\in E_i}\left(\frac{d(u)d(v)}{d(u)+d(v)}\right)$$
$$=\left(\frac{2\times2}{2+2}\right)(6n)+\left(\frac{2\times3}{2+3}\right)(12n-12)+\left(\frac{3\times3}{3+3}\right)(27n^2-51n+24)$$
$$=\frac{1}{10}[405n^2-561n+216].$$

## 4. Bond Additive Molecular Descriptors of Hexa-peri-hexabenzocoronene (HBC)

**Theorem 4.1** Let $G$ be a Hexa-peri-hexabenzocoronene (HBC). Then

1. $RLI(G)=32.58689292n^2-49.53341838n+19.82885112.$
2. $SLI(G)=56.59962n^2-74.35207n+27.74276.$
3. $ISLI(G)=(50.77802n^2-56.55225+19.98063)/3.94241.$
4. $MLI(G)=4.866n-4.866.$
5. $MLSI(G)=8.7168n-8.7168.$
6. $MII(G)=2n-2.$
7. $MIRI(G)=(6(\sqrt{6}-2)n-6(\sqrt{6}-2))/\sqrt{3}.$
8. $MRI(G)=12(-\sqrt{2}+\sqrt{3})n-12(-\sqrt{2}+\sqrt{3}).$
9. $MDI(G)=12n-12.$
10. $MHI(G)=(3n-3)/2.$
11. $MMRI(G)=27n^2-(45-4\sqrt{6})n-4\sqrt{6}+24.$
12. $MMRDI(G)=(27\sqrt{3}n^2+6\sqrt{2}-39\sqrt{3}n+6\sqrt{12})/\sqrt{2}.$
13. $MMDI(G)=27n^2-27n+6.$
14. $MMSDI(G)=27n^2-18n-3.$
15. $SDDI(G)=54n^2-64n+22.$

Proof.

$$RLI(G)=\sum_{uv\in E(G)}lnd_G(u)lnd_G(v)$$
$$=(ln2\times ln2)(6n)+(ln2\times ln3)(12n-12)$$
$$+(ln3\times ln3)(27n^2-51n+24)$$
$$=32.58689292n^2-49.53341838n+19.82885112.$$
$$SLI(G)=\sum_{uv\in E(G)}\sqrt{ln(d_u)}+\sqrt{ln(d_v)}$$
$$=\left[\sqrt{ln(2)}+\sqrt{ln(2)}\right](6n)+\left[\sqrt{ln(2)}+\sqrt{ln(3)}\right](12n-12)$$
$$+\left[\sqrt{ln(3)}+\sqrt{ln(3)}\right](27n^2-51n+24)$$
$$=56.59962n^2-74.35207n+27.74276.$$
$$ISLI(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{ln(d_u)}+\sqrt{ln(d_v)}}$$
$$=\left[\frac{1}{\sqrt{ln(2)}+\sqrt{ln(2)}}\right](6n)+\left[\frac{1}{\sqrt{ln(2)}+\sqrt{ln(3)}}\right](12n-12)$$

$$+\left[\frac{1}{\sqrt{ln(3)}+\sqrt{ln(3)}}\right](27n^2-51n+24)$$
$$=(50.77802n^2-56.55225+19.98063)/3.94241.$$
$$MLI(G)=\sum_{uv\in E(G)}|lnd_u-lnd_v|$$
$$=|ln2-ln2|(6n)+|ln2-ln3|(12n-12)$$
$$+|ln3-ln3|(27n^2-51n+24)$$
$$=4.866n-4.866.$$
$$MLSI(G)=\sum_{uv\in E(G)}|ln^2d_u-ln^2d_v|$$
$$=|ln^22-ln^22|(6n)+|ln^22-ln^23|(12n-12)$$
$$+|ln^23-ln^23|(27n^2-51n+24)$$
$$=8.7168n-8.7168.$$
$$MII(G)=\sum_{uv\in E(G)}\left|\frac{1}{d_u}-\frac{1}{d_v}\right|$$
$$=\left|\frac{1}{2}-\frac{1}{2}\right|(6n)+\left|\frac{1}{2}-\frac{1}{3}\right|(12n-12)+\left|\frac{1}{3}-\frac{1}{3}\right|(27n^2-51n+24)$$
$$=2n-2.$$
$$MIRI(G)=\sum_{uv\in E(G)}\left|\frac{1}{\sqrt{d_u}}-\frac{1}{\sqrt{d_v}}\right|$$
$$=\left|\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{2}}\right|(6n)+\left|\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right|(12n-12)$$
$$+\left|\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{3}}\right|(27n^2-51n+24)$$
$$=(6(\sqrt{6}-2)n-6(\sqrt{6}-2))/\sqrt{3}.$$
$$MRI(G)=\sum_{uv\in E(G)}|\sqrt{d_u}-\sqrt{d_v}|$$
$$=|\sqrt{2}-\sqrt{2}|(6n)+|\sqrt{2}-\sqrt{3}|(12n-12)$$
$$+|\sqrt{3}-\sqrt{3}|(27n^2-51n+24)$$
$$=12(-\sqrt{2}+\sqrt{3})n-12(-\sqrt{2}+\sqrt{3}).$$
$$MDI(G)=\sum_{uv\in E(G)}|d_u-d_v|$$
$$=|2-2|(6n)+|2-3|(12n-12)+|3-3|(27n^2-51n+24)$$
$$=12n-12.$$
$$MHI(G)=\sum_{uv\in E(G)}\left|\left(\frac{1}{2}\right)^{d_u}-\left(\frac{1}{2}\right)^{d_v}\right|$$
$$=\left|\left(\frac{1}{2}\right)^2-\left(\frac{1}{2}\right)^2\right|(6n)+\left|\left(\frac{1}{2}\right)^2-\left(\frac{1}{2}\right)^3\right|(12n-12)$$
$$+\left|\left(\frac{1}{2}\right)^3-\left(\frac{1}{2}\right)^3\right|(27n^2-51n+24)$$
$$=(3n-3)/2.$$
$$MMRI(G)=\sum_{uv\in E(G)}\sqrt{\frac{min(d_u,d_v)}{max(d_u,d_v)}}$$
$$=\sqrt{\frac{min(2,2)}{max(2,2)}}(6n)+\sqrt{\frac{min(2,3)}{max(2,3)}}(12n-12)$$
$$+\sqrt{\frac{min(3,3)}{max(3,3)}}(27n^2-51n+24)$$
$$=27n^2-(45-4\sqrt{6})n-4\sqrt{6}+24.$$
$$MMRDI(G)=\sum_{uv\in E(G)}\sqrt{\frac{max(d_u,d_v)}{min(d_u,d_v)}}$$

$$= \sqrt{\frac{max(2,2)}{min(2,2)}}(6n) + \sqrt{\frac{max(2,3)}{min(2,3)}}(12n - 12)$$
$$+ \sqrt{\frac{max(3,3)}{min(3,3)}}(27n^2 - 51n + 24)$$
$$= (27\sqrt{3}n^2 + 6\sqrt{2} - 39\sqrt{3}n + 6\sqrt{12})/\sqrt{2}.$$
$$MMDI(G) = \sum_{uv\in E(G)} \frac{max(d_u,d_v)}{min(d_u,d_v)}$$
$$= \frac{max(2,2)}{min(2,2)}(6n) + \frac{max(2,3)}{min(2,3)}(12n - 12) + \frac{max(3,3)}{min(3,3)}(27n^2 - 51n + 24)$$
$$= 27n^2 - 27n + 6.$$
$$MMSDI(G) = \sum_{uv\in E(G)} \left(\frac{max(d_u,d_v)}{min(d_u,d_v)}\right)^2$$
$$= \left(\frac{max(2,2)}{min(2,2)}\right)^2 (6n) + \left(\frac{max(2,3)}{min(2,3}\right)^2 (12n - 12)$$
$$+ \left(\frac{max(3,3)}{min(3,3)}\right)^2 (27n^2 - 51n + 24)$$
$$= 27n^2 - 18n - 3.$$
$$SDDI(G) = \sum_{uv\in E(G)} \left[\frac{min(d_u,d_v)}{max(d_u,d_v)} + \frac{max(d_u,d_v)}{min(d_u,d_v)}\right]$$
$$= \left[\frac{min(2,2)}{max(2,2)} + \frac{max(2,2)}{min(2,2)}\right](6n)$$
$$+ \left[\frac{min(2,3)}{max(2,3)} + \frac{max(2,3)}{min(2,3)}\right](12n - 12)$$
$$+ \left[\frac{min(3,3)}{max(3,3)} + \frac{max(3,3)}{min(3,3)}\right](27n^2 - 51n + 24)$$
$$= 54n^2 - 64n + 22.$$

The graphical representation of various degree-based topological indices of Hexa-peri-hexabenzocoronene is depicted in Figure 2 and Figure 3.

**Table 4.** The computed numerical value for degree-based indices.

| n | R(G) | RR(G) | RRR(G) | $M_1$(G) | $M_2$(G) | RM(G) |
|---|---|---|---|---|---|---|
| 1 | 3 | 12 | 6 | 24 | 24 | 6 |
| 2 | 21 | 143 | 89 | 288 | 390 | 156 |
| 3 | 57 | 437 | 280 | 876 | 1242 | 522 |
| 4 | 111 | 892 | 579 | 1788 | 2580 | 1104 |
| 5 | 183 | 1510 | 986 | 3024 | 4404 | 1902 |
| 6 | 272 | 2289 | 1501 | 4584 | 6714 | 2916 |
| 7 | 380 | 3230 | 2124 | 6468 | 9510 | 4146 |
| 8 | 506 | 4334 | 2855 | 8676 | 12792 | 5592 |
| 9 | 650 | 5599 | 3694 | 11208 | 16560 | 7254 |
| 10 | 812 | 7027 | 4641 | 14064 | 20814 | 9132 |

**Table 5.** The computed numerical value for degree-based indices.

| n | HM(G) | AZ(G) | ABC(G) | H(G) | SC(G) | GA(G) | ISI(G) |
|---|---|---|---|---|---|---|---|
| 1 | 96 | 48 | 4 | 3 | 3 | 6 | 6 |
| 2 | 1572 | 534 | 37 | 21 | 24 | 54 | 71 |
| 3 | 4992 | 1635 | 106 | 57 | 66 | 156 | 218 |
| 4 | 10356 | 3350 | 210 | 110 | 131 | 311 | 445 |
| 5 | 17664 | 5681 | 351 | 182 | 218 | 521 | 754 |
| 6 | 26916 | 8628 | 528 | 272 | 327 | 785 | 1143 |
| 7 | 38112 | 12189 | 741 | 380 | 457 | 1103 | 1613 |
| 8 | 51252 | 16365 | 989 | 506 | 610 | 1474 | 2165 |
| 9 | 66336 | 21156 | 1274 | 649 | 785 | 1900 | 2797 |
| 10 | 83364 | 26563 | 1595 | 811 | 982 | 2380 | 3511 |

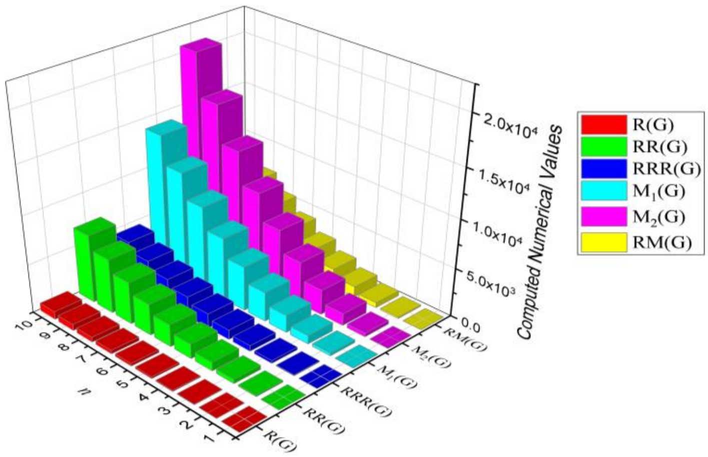


**Figure 2.** Graphical representation of degree-based indices

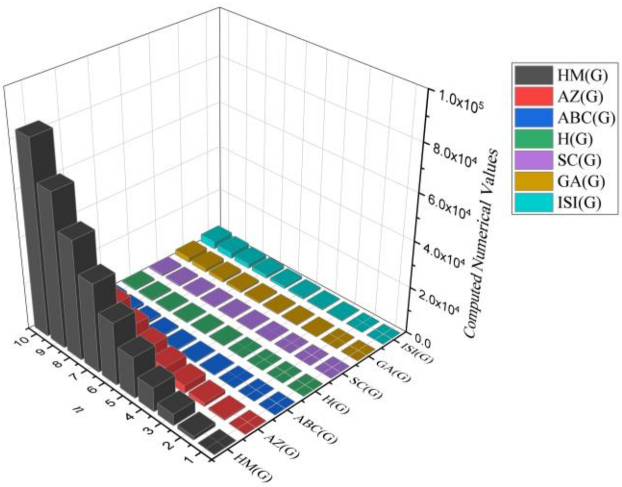


**Figure 3.** Graphical representation of degree-based indices.

The graphical representation of Bond Additive Molecular Descriptors of Hexa-peri-hexabenzocoronene is depicted in Figure 4 and Figure 5.

**Table 6.** The computed numerical value for bond additive.

| n | RLI(G) | SLI(G) | ISLI(G) | MLI(G) | MLSI(G) | MII(G) | MIRI(G) |
|---|---|---|---|---|---|---|---|
| 1 | 3 | 10 | 4 | 0 | 0 | 0 | 0 |
| 2 | 51 | 105 | 42 | 5 | 9 | 2 | 2 |
| 3 | 165 | 314 | 107 | 10 | 17 | 4 | 3 |
| 4 | 343 | 636 | 197 | 15 | 26 | 6 | 5 |
| 5 | 587 | 1071 | 313 | 19 | 35 | 8 | 6 |
| 6 | 896 | 1619 | 454 | 24 | 44 | 10 | 8 |
| 7 | 1270 | 2281 | 622 | 29 | 52 | 12 | 9 |
| 8 | 1709 | 3055 | 815 | 34 | 61 | 14 | 11 |
| 9 | 2214 | 3943 | 1034 | 39 | 70 | 16 | 12 |
| 10 | 2783 | 4944 | 1279 | 44 | 78 | 18 | 14 |

**Table 7.** The computed numerical value for bond additive.

| n | MRI(G) | MDI(G) | MHI(G) | MMRI(G) | MMRDI(G) | MMDI(G) | MMSDI(G) | SDDI(G) |
|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 0 | 6 | 6 | 6 | 6 | 12 |
| 2 | 4 | 12 | 2 | 52 | 57 | 60 | 69 | 110 |
| 3 | 8 | 24 | 3 | 152 | 175 | 168 | 186 | 316 |
| 4 | 11 | 36 | 5 | 305 | 359 | 330 | 357 | 630 |
| 5 | 15 | 48 | 6 | 513 | 609 | 546 | 582 | 1052 |
| 6 | 19 | 60 | 8 | 775 | 925 | 816 | 861 | 1582 |
| 7 | 23 | 72 | 9 | 1091 | 1307 | 1140 | 1194 | 2220 |

| n | MRI(G) | MDI(G) | MHI(G) | MMRI(G) | MMRDI(G) | MMDI(G) | MMSDI(G) | SDDI(G) |
|---|---|---|---|---|---|---|---|---|
| 8 | 27 | 84 | 11 | 1461 | 1755 | 1518 | 1581 | 2966 |
| 9 | 31 | 96 | 12 | 1884 | 2269 | 1950 | 2022 | 3820 |
| 10 | 34 | 108 | 14 | 2362 | 2850 | 2436 | 2517 | 4782 |

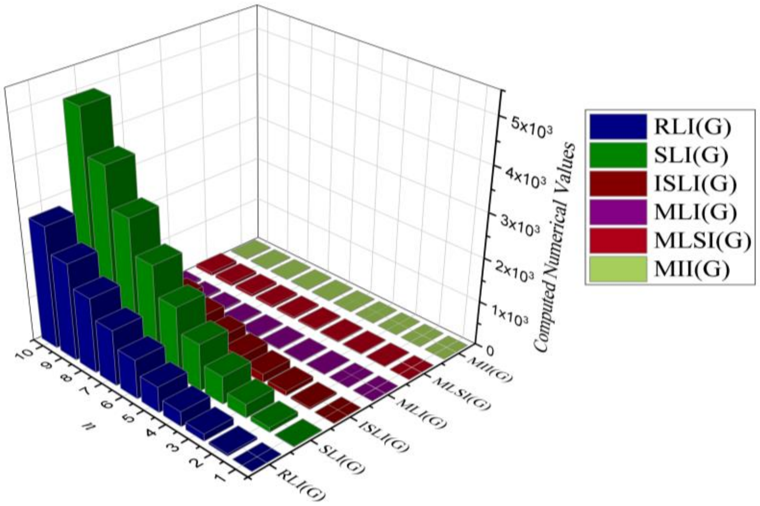


**Figure 4.** Graphical representation of bond additive.

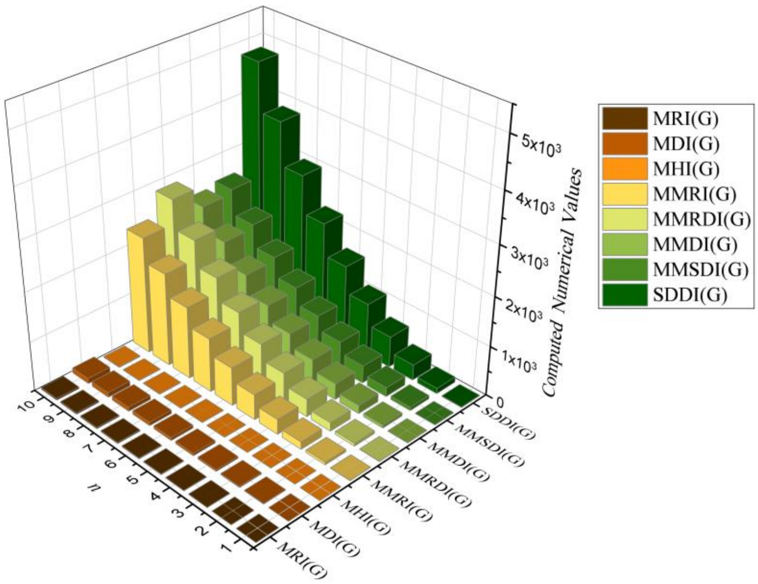


**Figure 5.** Graphical representation of bond additive.

## 5. Conclusions

In this paper, we have given the close expression of the Randic′, Reciprocal Randic′, Reduced reciprocal Randic′, First Zagreb, Second Zagreb, Reduced Second Zagreb, Hyper Zagreb, Augmented Zagreb, Atom bond connectivity, Harmonic, Sum-connectivity, Geometric arithmetic, Inverse sum indeg, First multiple Zagreb, Second multiple Zagreb indices and Bond additive of Hexa-peri-hexabenzocoronene.

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## Conflicts of Interest

The authors declare no conflict of interest.

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